Journal of Structural Geology, Vol. 10, No. 8, pp. 771 to 778, 1988
Printed in Great Britain

0191-8141/88 $03.00 + 0.00

Simulation of fabric development in recrystallizing aggregates—I. Description of the model

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(*Received* 30 *August* 1987; *accepted in revised form* 20 *June* 1988)

Abstract—A new computer simulation of the development of grain shape and crystallographic preferred orientations in dynamically recrystallizing aggregates is presented. This model is based on a uniform array of points, each of which represents a small area of crystal. This model combines homogeneous strains, simplified versions of the lattice rotations predicted by Taylor–Bishop–Hill theory, mobile grain boundaries and the nucleation of subgrains. It allows the progressive development of the fabrics and microstructures to be followed. The limitations of the simplifying assumptions used in this model are discussed.

INTRODUCTION

IT HAS long been recognized that there is some interplay between dynamic recrystallization and lattice rotations during fabric development (Kamb 1972, Duval 1981, Bouchez *et al.* 1983, Urai *et al.* 1986, Karato 1987); however, the exact nature of this relationship has been unclear. Current models of fabric development are solely based on the lattice rotations associated with crystal slip. Etchecopar's (1977) model did involve the bisection of grains in locked orientations; however this more properly modeled a fracturing rather than a recrystallization process. Recently Etchecopar & Vasseur (1987) have extended Etchecopar's (1977) model to allow more than one slip system to operate, and they included an explicit attempt to simulate the effects of recrystallization by resetting the grain shape to a foam texture at periodic intervals. Since this does not mimic any specific recrystallization processes, their study cannot investigate the relative roles of these processes in grain shape and crystallographic fabric development.

The goal of this study was to develop a simple computer simulation that could analyse the coupling of dynamic recrystallization processes and internal lattice rotations. The basis for the simulation is presented in this paper, and the results of a number of example runs are presented in a companion paper (Jessell 1988).

BASIS OF PRESENT MODEL

In recent years metallurgists have developed a number of Monte Carlo simulations of static grain growth and primary recrystallization in two dimensions (Anderson *et al.* 1984, Ceppie & Nasello 1984, Fradkov *et al.* 1985, Soares *et al.* 1985, Yabushita *et al.* 1985, Saetre *et al.* 1986). The most successful of these use a system of regularly spaced points (Anderson *et al.* 1984, for example), with each point having a specific crystallographic orientation (Fig. 1). Two neighbouring points which have the same orientation are considered to be part of the same grain, and two points with different orientations are separated by a grain boundary. The results of the grain growth simulations which are least dependent on the geometry of the array of points were found using a triangular array, and that is the pattern adopted here. By manipulating the positions and orientations associated with each point it is possible to model not only grain growth, but also several deformation processes. A flow chart that describes the simulation is shown in Fig. 2, and in the following sections each element of the simulation will be explained.

FABRIC INITIALIZATION

The original triangular array consists of a 100 × 100 set of points forming a rectangle whose sides are in the ratio of 1 : 1.15. Each point in this array is initially assigned a lattice orientation such that the array is divided up into

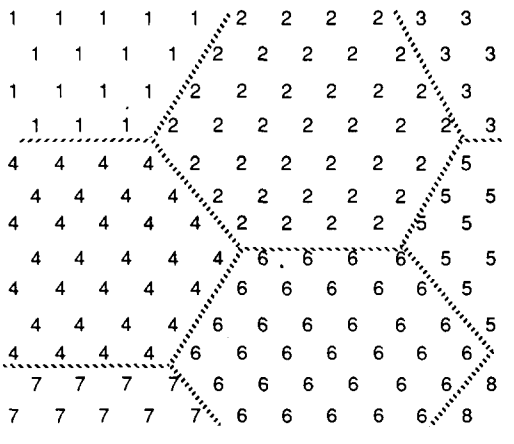

Fig. 1. Triangular array of points, which forms the basis of the model. Numbers refer to crystallographic orientations and the distribution of these numbers defines grain shapes. Grain 2 is a complete hexagonally-shaped grain with the standard initial grain size of 37 units.

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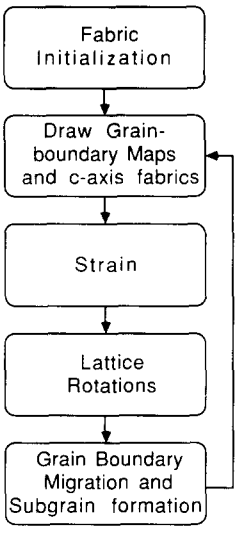

Fig. 2. Flow chart showing the relationship between the basic elements of the model. Refer to text for details of each element.

areas of equal orientation ('grains') with each grain consisting of 37 points. This number will henceforth be referred to as a grain size of 37 units. This model only considers one lattice orientation, here the c-axis of a trigonal or hexagonal material (such as quartz or ice, respectively) since the simple treatment of straining, lattice rotations and stored energy levels does not justify a more sophisticated approach. Each grain is randomly assigned an orientation, and the initial state consists of 300 grains (Fig. 3a), some of which are truncated by the borders of the array.

At the start of the simulation the conditions of deformation are set, and they remain constant throughout an individual run. Once the initial grain configuration has been set, the simulation consists of the iterative repetition of four syn-deformational processes: (1) redistribution of points to simulate strain; (2) reorientation of the crystallographic orientations of grains due to slip; (3) grain boundary migration; and (4) the nucleation of subgrains. Before each iteration a map of the grain boundaries is produced, together with the associated c-axis fabric diagrams.

STRAIN INCREMENT

The simulation of an increment of homogeneous strain is accomplished using different principles for simple shear and axially symmetric flattening. These are described separately.

Simple shear

Progressive dextral simple shear is approximated by shifting successive rows of points in the array to the left. The shear strain, γ, for one iteration was set at 0.19, which corresponds to a shortening of 9.95%. Since continuity within the model can only be maintained by shifting rows an integral number of positions to the left, a shear strain of 0.19 is distributed through 100 rows by taking up the shear as a shift of one position across 19 randomly chosen rows. By ensuring that the rows which take up the strain are relatively equally spaced, the

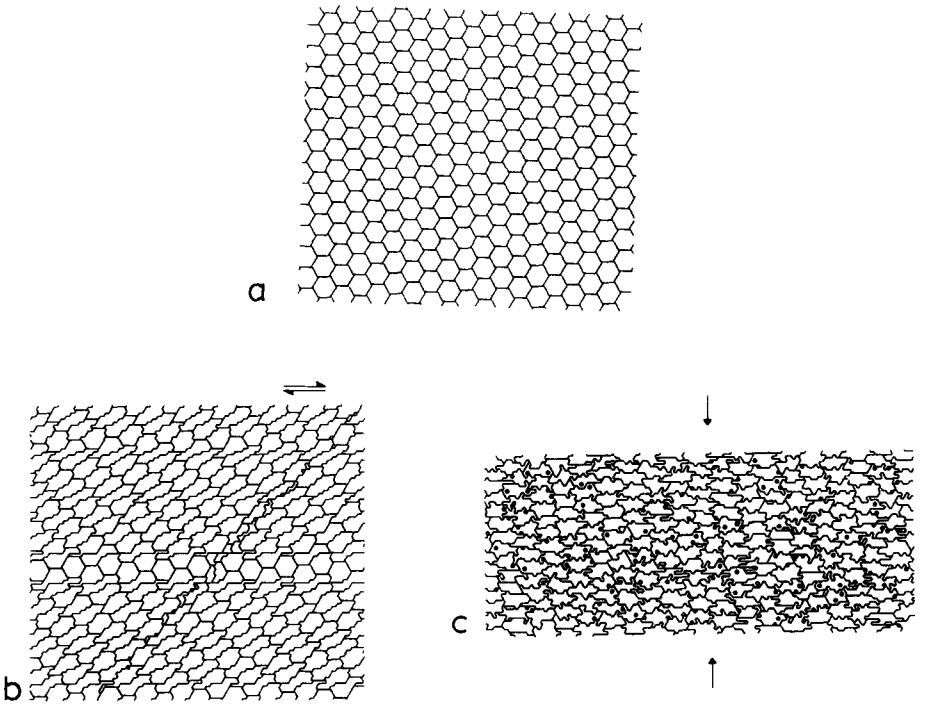

Fig. 3. (a) Configuration of grain boundaries in undeformed state. (b) The same grains deformed to a bulk shear strain of 0.95, with no recrystallization. The finer grains forming an oblique line are the edge grains in the initial fabric. (c) The same grains as in (a) axisymmetrically shortened by 38%, with no recrystallization. Notice the inherent area loss and the unwanted dissection of grains that results in this case.

strain is quite well distributed after five increments (Fig. 3b). Some grain break-up may occur at high strains purely as a result of the somewhat inhomogeneous straining induced by the strain algorithm.

Since shifting points to the left has the effect of moving material beyond the original boundaries of the array on the left and leaving empty space on the right, the vertical boundaries of the array are periodic, so that material that disappears off the left reappears on the right.

Axially-symmetric flattening

For increments of axially-symmetric flattening, a more complex method had to be used. Following the visualization of Bayly (1985), pure shear is seen as the removal of material along one set of planes and its addition along an orthogonal set of planes. To this end, points are randomly removed from each column of points, and then points are randomly added to each of the reduced number of rows. The added points are assigned the same orientation as their neighbours to the left. The main weakness of this method lies in the triangular nature of the array, since the points do not lie in true columns. This results in a much greater disruption of the arrangement of points than for simple shear (Fig. 3c), although it still results in a rough approximation to the geometry of axial compression. Average shortening rates of 9% per iteration were used.

LATTICE ROTATIONS

This model uses the reorientation trajectories for quartz *c*-axes predicted by Taylor–Bishop–Hill theory (Lister *et al.* 1978) as the basis for calculating the new orientations of grains after a given increment of deformation. Although Taylor–Bishop–Hill (TBH) theory requires that the full crystallographic orientation of the grain be specified, as a simplification the present model only considers the *c*-axis orientation. Therefore the *c*-axis rotations calculated in this simulation are not those predicted by TBH theory, but are gross simplifications of those predictions. Reorientation functions were developed which mimic the overall patterns of

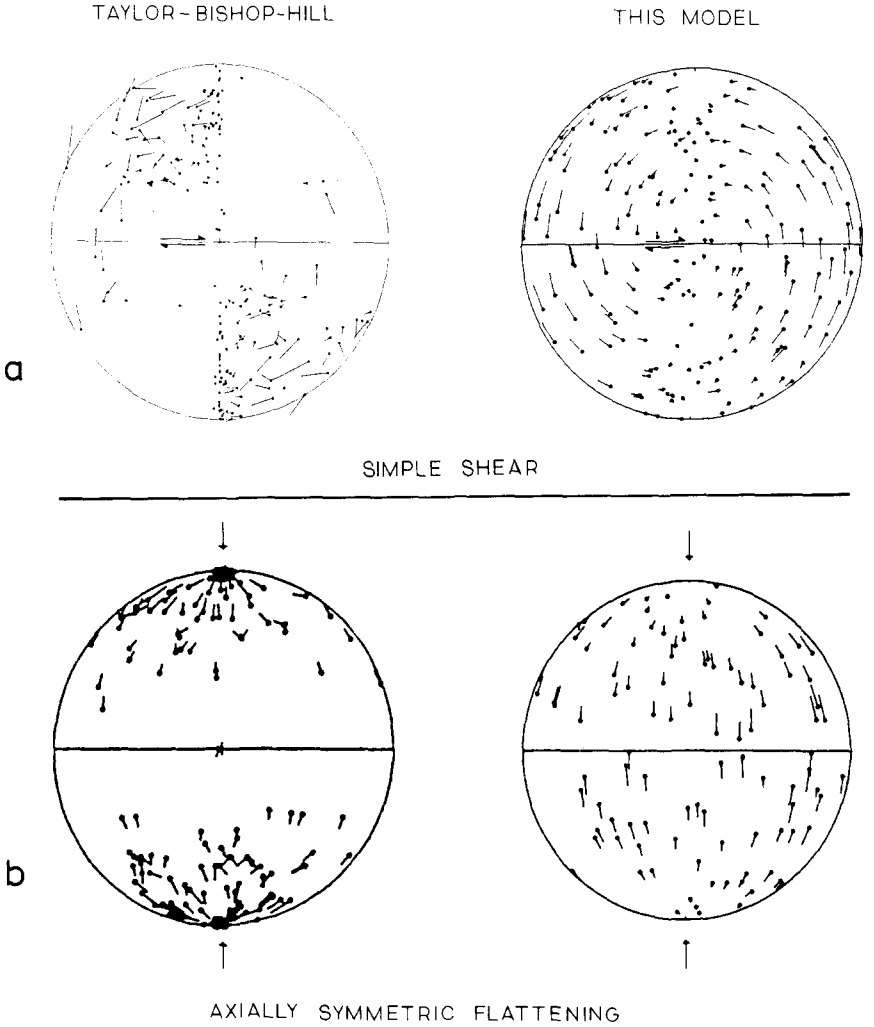

Fig. 4. Comparison of the lattice rotations predicted by Taylor–Bishop–Hill theory for quartz and the simplified versions used in this model. (a) In simple shear, for shear strains of 0.2 (Urai *et al.* 1986) and 0.19, respectively. (b) In axisymmetric flattening, for shortenings of 10% (Lister & Paterson 1979) and 9%, respectively. Equal-area lower-hemisphere projections. Points are *c*-axis orientations before deformation, the strokes show the amount and direction of *c*-axis rotation.

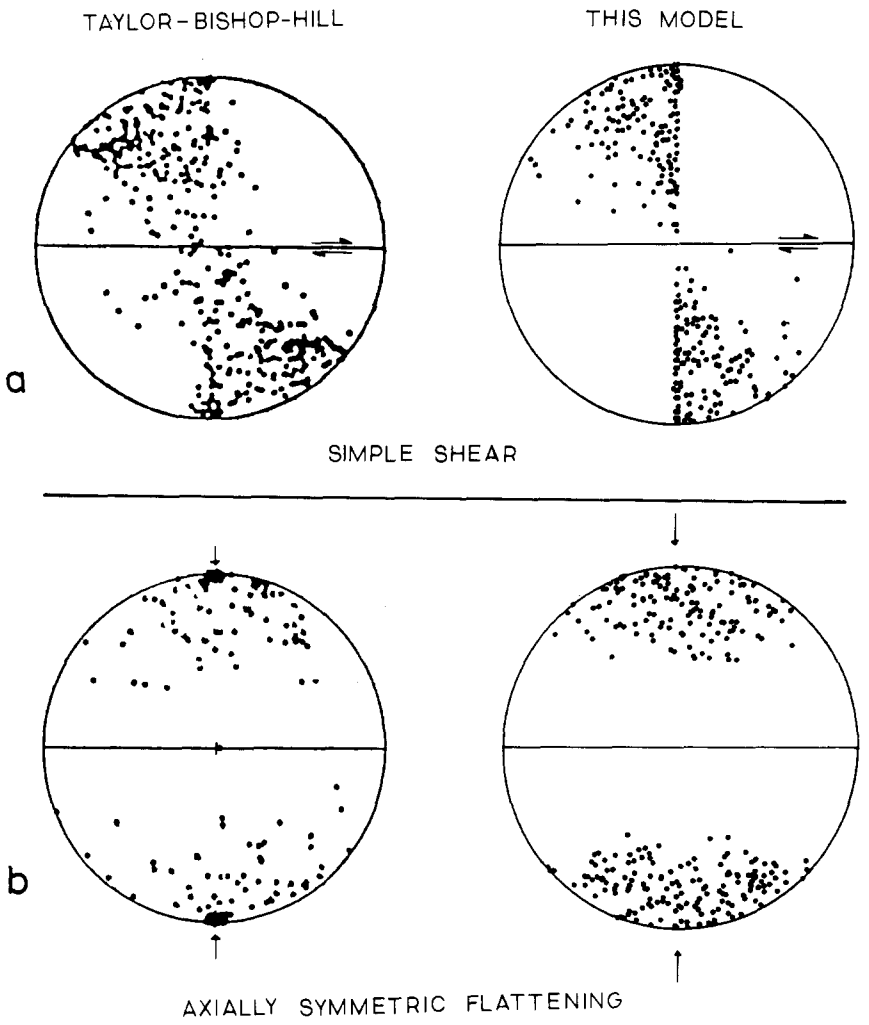

Fig. 5. Comparison of the *c*-axis fabrics that develop using Taylor–Bishop–Hill theory for quartz and the simplified lattice rotations used in this model. (a) In simple shear, for shear strains of 3.0 (Lister & Paterson 1979) and 3.04, respectively. (b) In axisymmetric flattening, for shortenings of 65% (Lister & Paterson 1979) and 65% this model. Equal-area lower-hemisphere projections.

c-axis reorientations predicted by TBH theory for quartz. In this model then, specification of the *c*-axis orientation and strain increment is sufficient information to predict the lattice reorientation.

Lister's work presents a number of alternative model 'quartzites' differentiated by the critical resolved shear stress values necessary to initiate slip on given glide planes (see for example Lister & Paterson 1979), so some choice from amongst these models had to be made. Lattice rotations based on critical resolved shear stress values from their work were chosen such that the *c*-axis fabrics that are predicted to develop have been measured in naturally or experimentally deformed quartzites, although this does not necessarily mean that the fabrics formed in the way TBH theory predicts. Quartz fabrics measured in simple shear regimes, both natural (Lister & Williams 1979) and experimental (Dell'Angello 1985) often produce Type I crossed girdles (Model B, Lister & Hobbs 1980), and that is the slip-induced pattern adopted here for simple shear. Tullis *et al.* (1973) subjected quartzites to axially-symmetric flattening, and the lower temperature, higher strain-rate runs produced single point maxima parallel to the compression axis, and that is the slip-induced pattern chosen for this strain geometry (Model A^1, fig. 10a, Lister & Paterson 1979).

TBH theory predicts that the magnitude of reorientation for a given orientation is proportional to the magnitude of the strain increment, so that this model must make some assumption about the size of the lattice rotations for a given strain increment. The average rate of lattice rotation for a given strain increment is taken from Lister & Hobbs (1980, fig. 17d). The lattice rotations predicted by TBH theory and this model's approximations for each strain geometry are shown in Fig. 4, and the resulting *c*-axis fabrics are compared in Fig. 5. It can be seen that there is a good correspondence between the *c*-axis fabrics that evolve, although no predictions are made for any other crystal axis.

RECRYSTALLIZATION

The two recrystallization processes simulated in this model are grain boundary migration and subgrain formation.

Grain boundary migration

The choice of driving force for grain boundary migration plays an important role in the evolution of fabrics in this model, so the reasons for this choice will be discussed in some detail. Based on my observations of dynamically recrystallizing octachloropropane (Jessell 1986), the stored energy of deformation is thought to be variable and related to both the crystallographic orientation of a grain with respect to the stress field and its internal strain state. TBH theory assumes a homogeneous strain state and heterogeneous stress state, whereas the formulation of the stored energy equations for this model assume a stress field with a uniform orientation. Hence I assume both roughly homogeneous stress and homogeneous strain.

Kallend & Huang (1984) have demonstrated orientation-dependent variations in the stored energy of deformation in cold-worked copper polycrystals, and their results suggest that grains well oriented for slip on a single slip system have lower stored energy levels. In contrast, for experimentally deformed dunites, Karato (1987) has shown that grains well oriented for slip actually have higher dislocation density levels. I feel that Karato's results are consistent with the orientation- and strain-dependent model presented in Jessell (1986), if the grains poorly oriented for slip are so resistant to deformation that they do not deform at all, although there is no direct evidence for this in Karato's experiments. In this model the orientations of lowest stored energy are assumed to be those which have major slip systems parallel to the maximum shear stress orientations, as also postulated by Urai & Humphreys (1981), Duval (1981) and Schmid & Casey (1986).

On this basis it is possible to create simple functions for the orientation dependent distribution of stored energy (E_{so}), given the observed slip systems for quartz. The functions used were, for simple shear:

$$E_{so} = \frac{1 + 2(1 - \cos(\varrho)\cos(2\phi))}{3}, \quad (1)$$

where ϱ is the plunge of the c-axis away from the plane of the model and ϕ is the plunge direction relative to the boundaries of the model; and for axisymmetric flattening:

$$E_{so} = \frac{1 + 2\cos(2\theta)}{3}, \quad (2)$$

where θ is the angle between the incremental shortening direction and the c-axis. E_{so} can thus vary between 1/3 and 1, so that even a perfectly oriented grain still has a significant stored energy level. In this study the effects of assuming that either the basal $\langle a \rangle$ or the prism $\langle a \rangle$ slip systems control the patterns of stored energy are investigated. This does not mean that the model assumes deformation by slip on a single system, merely that grains that deform in certain single slip orientations will have lower levels of stored energy than those that do not. The predicted patterns of stored energy for these slip systems undergoing increments of simple shear and axially symmetric flattening are shown in Fig. 6. These distributions assume that the stored energy of deformation is the same for a single basal plane $\langle a \rangle$ direction slip as for a combination of slips on two basal plane $\langle a \rangle$ directions (and similarly for one and two prism plane $\langle a \rangle$ direction slips).

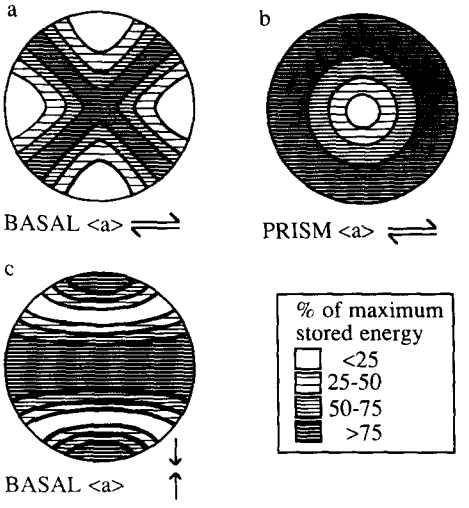

Fig. 6. The orientation-dependent distributions of the stored energy of deformation assumed in this model, contoured on equal-area lower-hemisphere projections. Each projection represents one combination of a deformation geometry with one controlling slip system. (a) Simple shear and basal $\langle a \rangle$. (b) Simple shear and prism $\langle a \rangle$. (c) Axisymmetric flattening and basal $\langle a \rangle$.

Since the strain is homogeneous in this model, variations in internal strain state only arise when considering grains of different ages, which in turn only arise when considering boundaries involving recently formed subgrains. New grains and subgrains are assumed to have no stored energy, but as they deform they asymptotically reach the stored energy level of old grains with the same orientation. The function used was:

$$E_s = E_{so}(1 - 0.5^t), \quad (3)$$

where E_{so} is the orientation-dependent stored energy from equation (1) or (2), and t is the number of increments since grain or subgrain formation. It is assumed that the material is perfectly annealed at the start of the simulation, so that there is an initial period of low grain boundary velocities.

Grain boundary migration is simulated for each iteration in the following manner. First a point is randomly selected from the array. This point is then compared with one of its six neighbours, again chosen at random. If the two points both have the same orientation, the local area is considered to be part of a grain interior, so no grain boundary exists. If the two points have different orientations, however small (Fig. 7a), the hypothetical stored energy for each point based on its age and orientation is calculated. These values can vary anywhere between 0 (for new grains) and 1 for very poorly oriented old grains. The difference between the two stored energy levels provides the driving force for grain boundary migration and is used as the probability of local reorien-

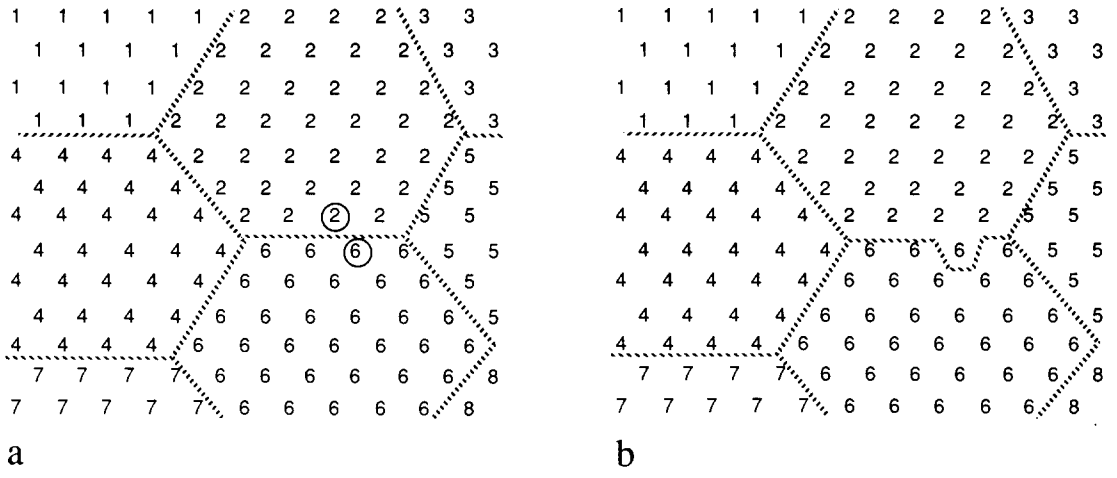

Fig. 7. Simulation of grain boundary migration. (a) Two neighbouring points (circled) are separated by an inferred grain boundary (dotted line), and are compared by the recrystallization algorithm. (b) The algorithm calculates that point 2 has a lower stored energy than point 6, and chooses whether to switch the orientation of point 6 to that of point 2 with a probability defined by the contrast in stored energy levels. In this case it chose to switch the orientation, and a grain boundary migration event has taken place.

tation of the higher stored energy point to the orientation of the lower stored energy point (Fig. 7b).

The whole process, starting with the random choice of a point in the array, is carried out a large number of times for each deformation increment, the actual number determining the mobility of the grain boundaries. A mobility of 1 is arbitrarily defined as carrying out this process 10,000 times for each increment of deformation, or on average once for each point in the array, increasing the mobility increases grain boundary velocities for a given driving force.

Since this model has unspecified spatial dimensions, apart from the lower grain size limit of a single point, an increase in grain boundary mobility is geometrically equivalent to a decrease in initial grain size, so the choice of mobilities is somewhat arbitrary, although the discrete nature of the points influences the smallest grain boundary bulge dimension. Direct evidence for grain boundary velocities in deforming polycrystals comes from experiments such as those of Urai (1983, in carnallite), Wilson & Russell-Head (1982, in ice) and Means (1983, in octachloropropane), and Tullis & Yund (1982) provide values for grain growth in quartz. In this model mobilities are chosen so that for a given strain, the dimensionless ratio of the average distance moved by a grain boundary to the grain size is within an order of magnitude of that seen in octachloropropane, as measured by the author (unpublished results).

Subgrain formation

In this model subgrains only form at grain boundaries, which excludes the type of intra-granular subgrain formation process reported by Etheridge (1975) and Bell (1979). When neighbouring points are compared during grain boundary migration modeling, and are found to have different orientations, there is in each case a finite probability that instead of a grain boundary event taking place, a subgrain is formed (Fig. 8). The rate of subgrain formation is controlled by this probability. There are

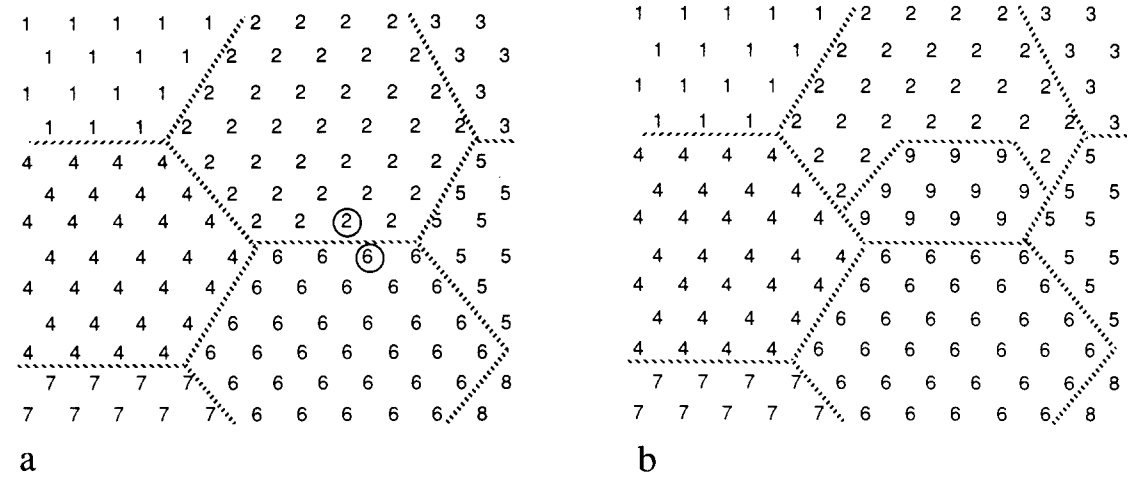

Fig. 8. Simulation of subgrain formation. (a) Two neighbouring points (circled) are separated by a grain boundary (dotted line), and are compared by the recrystallization algorithm. (b) According to a preset probability the algorithm chooses whether to nucleate a subgrain, as it does in this case, and part of the first chosen grain is replaced by material with a new orientation.

two further restrictions to the formation of subgrains: the stored energy of the host grain must reach a threshold level of 0.2, and the host grain must have an area of at least 20 units. The initial size of the subgrains is about 9 units, and their future growth and lattice reorientations are governed by the same principles as original grains. The new subgrain is superimposed only over the host grain, such that all points that lie within a hexagon centered over the chosen point, with sides of three points, become part of the subgrain. As a result there is some variation in initial subgrain size dependent on the local geometry of the grain boundary. The *c*-axis orientation of the subgrain is randomly chosen from within a 10° angular separation of the host grain.

DISCUSSION

As in any simulation, a set of simplifying assumptions had to be made in order to reduce the problem to manageable proportions. Some of the limitations and foreseeable consequences of these assumptions are discussed below.

Strain heterogeneity

The problem of heterogeneous deformation is not considered in this model. Mancktelow (1981) has demonstrated that strain contrasts can be related to grain orientations in a naturally deformed quartzite. Since the simplified lattice rotations are based on TBH theory, which assumes homogeneous strain, this model does likewise. The introduction of heterogeneous strain would be a much more complex problem, even if it would be potentially more rewarding. The exclusion of the interaction between intra-grain strains and lattice orientations is a particular weakness of this simulation. In principle it may be possible to replace the strain algorithms with a finite-difference approach, although as yet this has not been attempted.

Lattice rotations

The inclusion of genuine TBH theory lattice rotations will greatly enhance the predictive powers of this model, since the full crystallographic description of preferred orientations could then be compared with natural and experimental examples. The inclusion of the real TBH model has now been carried out and the results will be the subject of a future paper.

The driving force for grain boundary migration

This model implies that the local stored energy levels are independent of the age structure of the grains. In fact, as has been shown by the experiments of Means (1983) and Urai (1983), material in different parts of the same grain can have been swept by grain boundaries at different stages of its history. Toriumi (1982) annealed naturally deformed peridotites at atmospheric pressure and observed the development of characteristic dislocation densities behind the migrating boundary. The introduction of local intra-grain histories would considerably complicate the analysis.

Another grain boundary phenomenon ignored by this simulation is the bimodal distribution of grain boundary velocities observed by Urai (1983) in experimentally deformed bischofite. The resolution of the array of points compared to grain sizes does not allow this phenomenon to be studied here, although the use of the whole array to simulate a bicrystal may make this feasible. The resolution of the underlying array determines the lower limits to grain size and grain boundary bulge wavelength, and again these microstructures could be better studied using a larger starting grain size.

It seems reasonable to relate the pattern of stored energy of deformation to the critical resolved shear stress values. Hence if temperature, strain rate and the partial pressure of H_2O affect the flow behaviour of quartz by changing critical resolved shear stress values as could be interpreted from the work of Tullis *et al.* (1973), Blacic (1975) and Hobbs (1985), these factors should also affect the patterns of stored energy, so that, in a more complete model, lattice reorientation patterns would systematically vary with changes in the patterns of stored energy.

Subgrain formation

The progressive misorientation of subgrains has been investigated by Guillope & Poirier (1979); however the process is not yet understood to the extent that specific predictions about the formation and interaction of subgrains can confidently be made, even for very simple deformations and grain boundary geometries. Gottstein *et al.* (1979) have demonstrated that subgrains in single crystals of copper deformed in tension have twin relationships with the host, and this may also apply to minerals (Avé Lallement 1978). Guillope & Poirier (1979), based on their experiments on salt, suggest that "nucleation in the classical sense probably does not exist", and no attempt was made here to introduce new completely random orientations, although this would be simple enough to do. Instead an upper limit of 10° was imposed on the initial misorientation of the subgrain, although further misorientation could occur due to the differing lattice rotation trajectories that the host and subgrain follow during subsequent deformation.

Extending the model

The model as it stands investigates one driving force for grain boundary migration, one type of subgrain formation, and one type of lattice rotation, and it may be worthwhile exploring other aspects of recrystallization. Using this type of model, three-dimensional static grain growth has been carried out by Anderson *et al.* (1985), and only minor differences between the behaviour of the two- and three-dimensional polycrystals was found, so it is probably not necessary to extend the present model to

three dimensions. Other aspects of grain boundary migration could also be modeled using slight variations of the basic model, for example the influence of a second phase has been investigated by Srolovitz *et al.* (1984). As these workers have shown, this type of model is flexible enough to allow many aspects of recrystallization processes to be analysed. One process clearly of interest in geological materials is the modification of deformation fabrics by post-tectonic annealing.

The value of this model, which primarily depends on the validity of the assumptions made in it, also needs to be tested by producing results which are consistent with observations from naturally and experimentally deformed rocks. This is the object of the companion paper (Jessell 1988) which compares fabrics predicted by this model with some previously reported examples.

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Note: Copies of the program described in this paper, reformulated to run on a Macintosh™ computer, may be obtained by sending a blank disk to the author.

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